Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptaeal1624

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC 01	ChemPort single article sales feature unavailable
NEWS	3	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS	4	APR 07	STN is raising the limits on saved answers
NEWS	5	APR 24	CA/CAplus now has more comprehensive patent assignee information
NEWS	6	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS	7	APR 28	CAS patent authority coverage expanded
NEWS	8	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS	9	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS	10	MAY 08	STN Express, Version 8.4, now available
NEWS	11	MAY 11	STN on the Web enhanced
NEWS	12	MAY 11	BEILSTEIN substance information now available on STN Easy
NEWS	13	MAY 14	DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format
NEWS	14	MAY 15	INPADOCDB and INPAFAMDB enhanced with Chinese legal status data
NEWS	15	MAY 28	CAS databases on STN enhanced with NANO super role in records back to 1992
NEWS	16	JUN 01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN customer agreement. This agreement limits use to scientific research. Use for software development or design, implementation of commercial gateways, or use of CAS and STN data in the building of commercial products is prohibited and may result in loss of user privileges

<12/04/2007> Erich Leese

and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:50:28 ON 22 JUN 2009

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.66	0.66

FILE 'REGISTRY' ENTERED AT 15:52:03 ON 22 JUN 2009

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JUN 2009 HIGHEST RN 1159253-26-5
DICTIONARY FILE UPDATES: 21 JUN 2009 HIGHEST RN 1159253-26-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

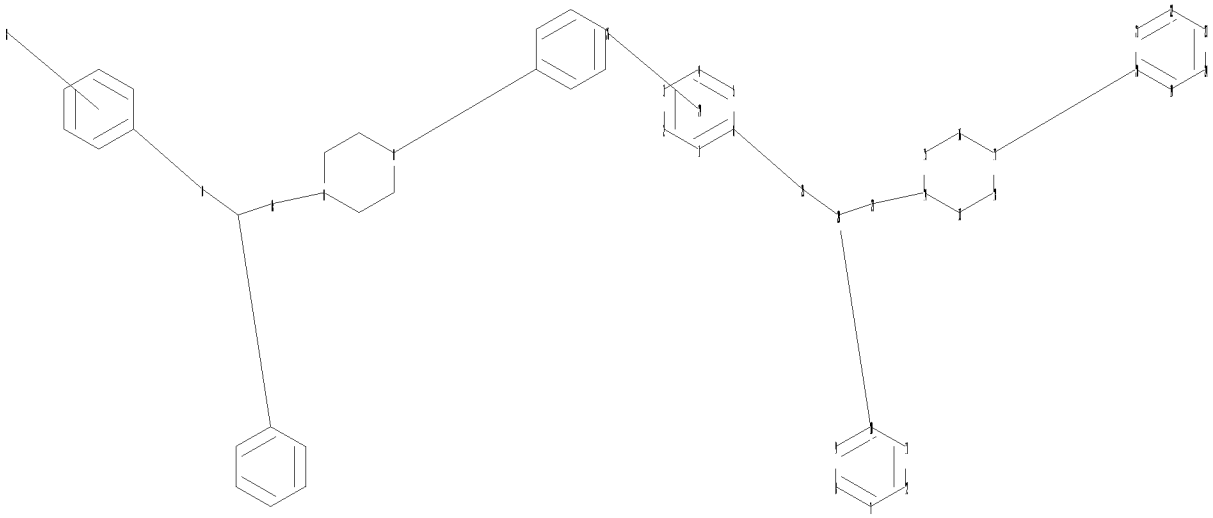
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10594105species.str



```
chain nodes :
25  26  27  28
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22  23
24
chain bonds :
6-25  10-28  14-27  17-20  25-28  27-28
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12  13-14  13-18
14-15  15-16  16-17  17-18  19-20  19-24  20-21  21-22  22-23  23-24
exact/norm bonds :
6-25  13-14  13-18  14-15  14-27  15-16  16-17  17-18  17-20  25-28  27-28
exact bonds :
10-28
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12  19-20  19-24
20-21  21-22  22-23  23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:Atom  22:Atom  23:Atom  24:Atom  25:CLASS  26:CLASS  27:CLASS  28:CLASS
 29:Atom



L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:53:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    11045 TO ITERATE

100.0% PROCESSED    11045 ITERATIONS                                 88 ANSWERS
SEARCH TIME: 00.00.01

L2           88 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   186.84     187.50
```

FILE 'CAPLUS' ENTERED AT 15:53:50 ON 22 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 22 Jun 2009 VOL 150 ISS 26
FILE LAST UPDATED: 21 Jun 2009 (20090621/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

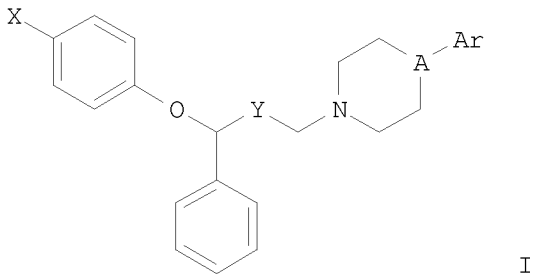
=> s l2 full
L3 2 L2

=> d ibib abs hitstr tot
THE ESTIMATED COST FOR THIS REQUEST IS 11.28 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

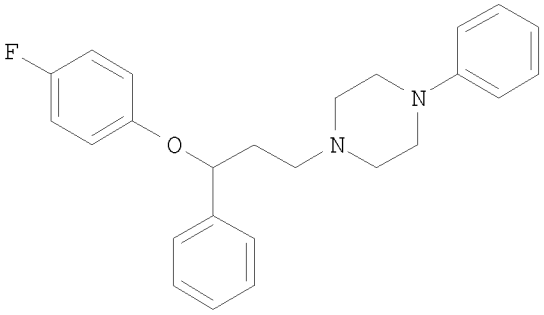
L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103625 CAPLUS
DOCUMENT NUMBER: 143:387060
TITLE: Preparation of piperazine or piperidine derivatives as serotonin reuptake inhibitors
INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey, James Michael
PATENT ASSIGNEE(S): Baylor University, USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005094896	A2	20051013	WO 2005-US10356	20050328
WO 2005094896	A3	20070503		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA				
EP 1732610	A2	20061220	EP 2005-730778	20050328
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
US 20080132514	A1	20080605	US 2007-594105	20070921
PRIORITY APPLN. INFO.:			US 2004-557069P P	20040326
			WO 2005-US10356 W	20050328

OTHER SOURCE(S): CASREACT 143:387060; MARPAT 143:387060
GI



I



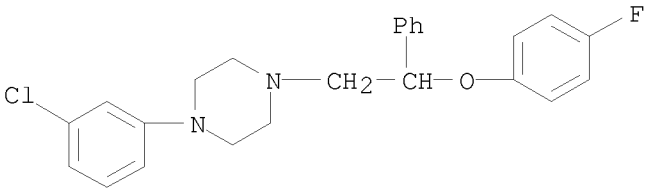
II

AB Title compds. I [X = F or CF3; Y = (CH2)n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [3H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC50 values in the range of 1.45 up to 9.56 μM. I as serotonin reuptake inhibitors should prove useful in the treatment of depression. Pharmaceutical composition comprising I are disclosed.

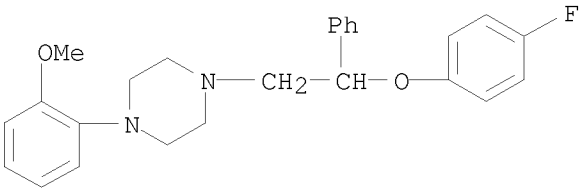
IT 691872-56-7P 691872-58-9P 691872-60-3P
691872-62-5P 691872-64-7P 691872-66-9P
866548-21-2P 866548-22-3P 866548-24-5P
866548-25-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperazine or piperidine derivs. as serotonin reuptake inhibitors)

RN 691872-56-7 CAPLUS

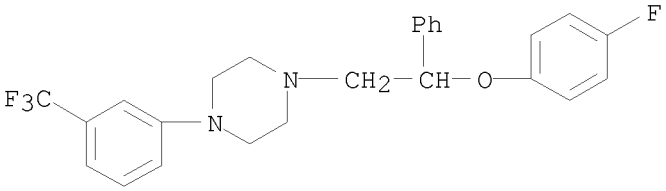
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



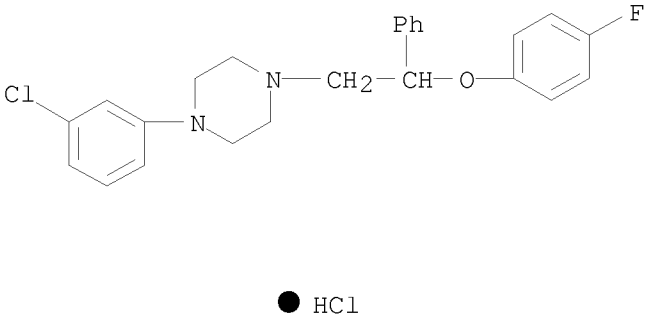
RN 691872-58-9 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 691872-60-3 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



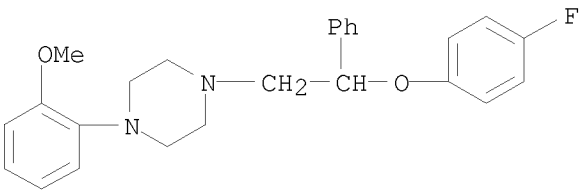
RN 691872-62-5 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

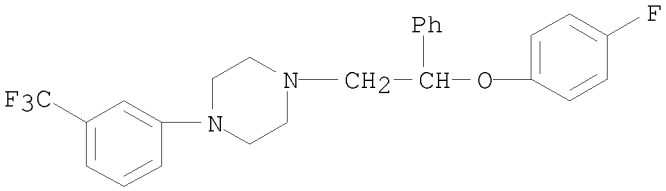
RN 691872-64-7 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



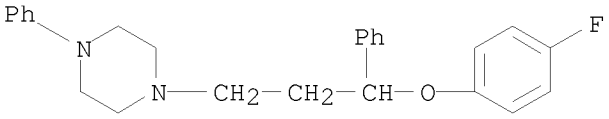
● HCl

RN 691872-66-9 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

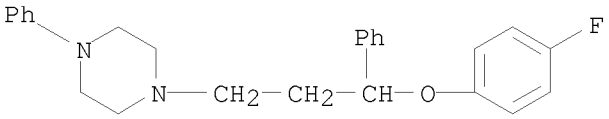


● HCl

RN 866548-21-2 CAPLUS
CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl- (CA INDEX NAME)

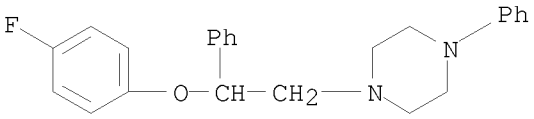


RN 866548-22-3 CAPLUS
CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)

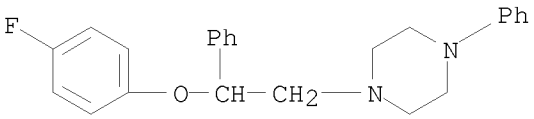


● HCl

RN 866548-24-5 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl- (CA INDEX NAME)



RN 866548-25-6 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



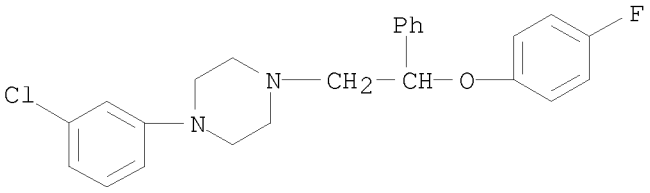
● HCl

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:170822 CAPLUS
DOCUMENT NUMBER: 140:417233
TITLE: Synthesis and biological evaluation of 2-(4-fluorophenoxy)-2-phenyl-ethyl piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile
AUTHOR(S): Dorsey, James M.; Miranda, Maria G.; Cozzi, Nicholas V.; Pinney, Kevin G.
CORPORATE SOURCE: Department of Chemistry and Biochemistry and The Center for Drug Discovery, Baylor University, Waco, TX, 76798-7348, USA
SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(6), 1483-1491
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:417233

AB Three new 2-(4-fluorophenoxy)-2-phenyl-Et piperazines, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-piperazine, and 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(3-trifluoromethylphenyl)-piperazine, modeled after the potent antidepressant fluoxetine and coupled with several functionalized piperazines, have been prepared by chemical synthesis as selective serotonin reuptake inhibitors (SSRIs) with a potentially improved adverse reaction profile. Typical SSRIs, although very effective in the treatment of depression, still face the troublesome side effect of sexual dysfunction. A number of pharmacol. agents-notably, drugs in the piperazine class-have been used to reverse SSRI-induced sexual dysfunction, and evidence for developing an improved SSRI by coupling a fluoxetine congener with the pharmacophore of a reversal agent holds promise. Preliminary data indicates that the hydrochloride (HCl) salts of piperazines exhibit single-site binding at the site of the serotonin reuptake transporter (SERT). However, each of the three compds. are much less potent than typical SSRIs, showing micromolar (μM) affinity for the SERT with IC50 values of 1.45 μM, 3.27 μM, and 9.56 μM, resp. Further biol. evaluation of piperazine compds. is needed before definitive conclusions can be made with regard to each compound's potential for use as an SSRI-type candidate which is devoid of sexual side effects. Nevertheless, the initial findings are quite encouraging, thus lending credence to the idea of hybridizing an SSRI congener with that of the pharmacophore of an agent known to reverse or treat SSRI-induced sexual dysfunction.

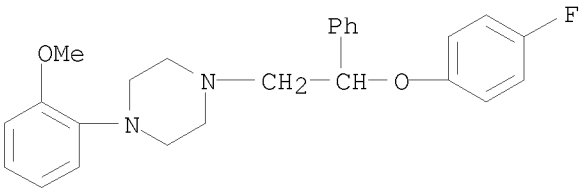
IT 691872-62-5P 691872-64-7P 691872-66-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)

RN 691872-62-5 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-, hydrochloride (1:1) (CA INDEX NAME)



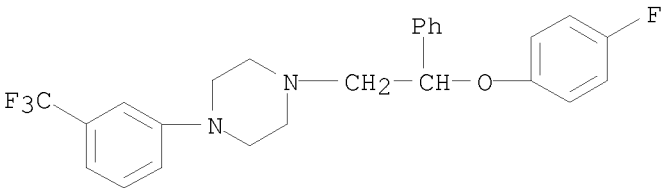
● HCl

RN 691872-64-7 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 691872-66-9 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

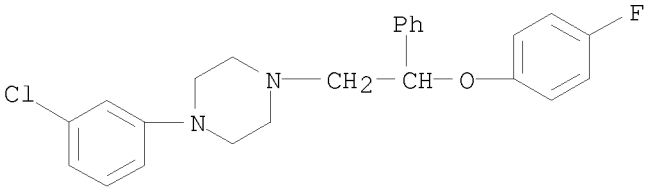


● HCl

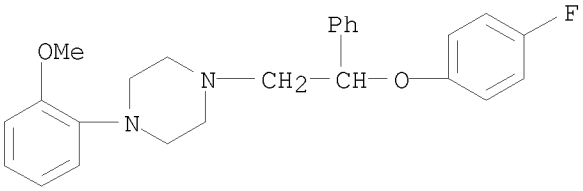
IT 691872-56-7P 691872-58-9P 691872-60-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)
RN 691872-56-7 CAPLUS

<12/04/2007> Erich Leese

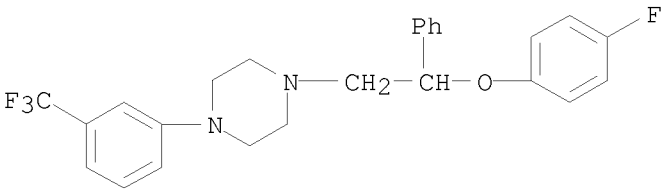
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



RN 691872-58-9 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 691872-60-3 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
=> d his

     (FILE 'HOME' ENTERED AT 15:50:28 ON 22 JUN 2009)

     FILE 'REGISTRY' ENTERED AT 15:52:03 ON 22 JUN 2009
L1             STRUCTURE UPLOADED
L2          88 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 15:53:50 ON 22 JUN 2009
L3           2 S L2 FULL

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    20.28     207.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -1.64      -1.64

STN INTERNATIONAL LOGOFF AT 16:04:47 ON 22 JUN 2009
```